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Electronic Properties of Various B-Doped Diamond (111)/Dye Molecule Interfaces

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Diamond is a widely known material for its many excellent properties. A B-doped diamond is an excellent p-type material for solar cell usage. It is considered as one of the strongest candidates for photovoltic electric generation. In the present investigation, the adsorption of different dye molecules onto H-terminated diamond (111) surfaces have been theoretically studied using Density Functional Theory (DFT) calculations. The diamond surfaces were B-doped in order to make them p-type semi-conducting. The choice of dyes was based on the match between the electronic structures of these H-terminated B-doped diamond surfaces and the respective dye molecules. The dye molecules in the present study include C26H13NO3S4(A), C35H37NO2S3(B), C34H38OS2(C), C32H36OS2(D) and C31H35S3Br(E).The main goal with the present study was thereby to investigate and compare the photo-voltaic efficiency of the various dyes when attached to B-doped and H-terminated diamond surfaces. The calculated absorption spectra in principle of the different dyes were shown to be located in the most intense part of the sunlight spectrum. The usage of a combination of these different dyes would hence, be an optimal choice in order to improve the light harvesting in a photovoltaic process.

Biography:

Karin Larsson is a Professor in Inorganic Chemistry at the Department of Materials Chemistry, Uppsala University, Sweden. She received a PhD in Chemistry in 1988. The research was directed towards investigation of molecular dynamic processes in solid hydrates by using solid state NMR spectroscopy. The scientific focus is on interpretation, understanding and prediction of the following processes/properties for both solid/gas interfaces, as well as for solid/liquid interfaces; i)CVD growth, ii)interfacial processes for renewable energy applications and iii)interfacial processes for e.g. bone regeneration (incl. biofunctionalisation of surfaces).